TITLE: Development and application of interatomic potentials for ultra high temperature ceramics (UHTC): ZrB2 and HfB2

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ABSTRACT BODY: Ultra high temperature ceramics (UHTC) including ZrB2 and HfB2 are characterized by high melting point, good strength, and reasonable oxidation resistance. These materials are of interest for use as sharp leading edges for hypersonic vehicles among other applications. Progress in computational modeling of UHTCs has been limited in part due to the absence of suitable interatomic potentials. We present a Tersoff style parameterization of such potentials for ZrB2 and HfB2 appropriate for atomistic simulations. Parameters are fit to data generated from ab initio calculations. The accuracy of the potentials is assessed against further ab initio data. As a first non-trivial application, molecular dynamics simulations are performed to evaluate the thermal conductivity of single crystals and the thermal resistance of high symmetry grain boundaries.

KEYWORDS: Multiscale Modeling, MD Simulation, Ab Initio Calculation, Thermal Conductivity, ZrB2, UHTC